Schedule for the **Computational Materials Workshop**
ORNL, Dec. 10-14, 2007.
Prof. Marco Buongiorno Nardelli, NCSU-ORNL

Monday, Dec. 10
9-10 Introduction to computational materials modeling and electronic structure
10-11 Theoretical background I: quantum mechanics
11-12 Theoretical background II: crystal symmetry and Bloch states
Lunch
2-3 Uniform electron gas: simple metals
3-4 Density Functional Theory I: Hohemberg-Kohn theorem, Kohn-Sham ansatz
4-5 Density Functional Theory II: Kohn-Sham equations and exchange-correlation functionals

Tuesday, Dec. 11
9-10 Atoms and pseudopotential theory
10-11 Plane wave calculations I - foundations
11-12 Plane wave calculations II - quantum-ESPRESSO
Lunch
2-3 Solution of the Kohn-Sham problem: iterative methods and algorithms
3-4 Software demonstrations and Q&A
4-5 Graphical User Interfaces: PWgui and XCrysDen

Wednesday, Dec. 12
Morning: Computational laboratory
Lunch
2-3 Orbital basis: LCAO and Tight Binding
3-4 Quantum chemical calculations I (lecturer TBA)
4-5 Quantum chemical calculations II (lecturer TBA)

Thursday, Dec. 13
9-10 Introduction to supercomputing at ORNL (lecturer Dr. Edo Apra', ORNL)
10-11 Electronic polarization and localization: Berry phases and Wannier functions (I)
11-12 Electronic polarization and localization: Berry phases and Wannier functions (II)
Lunch
2-3 Density Functional Perturbation Theory
3-4 Electronic excitations
4-5 The Car-Parrinello method

Friday, Dec. 14
9-10 Introduction to electronic transport I (lecturer Dr. Vincent Meunier, ORNL)
10-11 Introduction to electronic transport II (lecturer Dr. Vincent Meunier, ORNL)
11-12 Q&A - concluding discussion